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Entanglement and quantum phase transition in alternating XY spin chain with next-nearest neighbouring interactions*

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By using the method of density-matrix renormalization-group to solve the different spin–spin correlation functions, the nearest-neighbouring entanglement (NNE) and the next-nearest-neighbouring entanglement (NNNE) of one-dimensional alternating Heisenberg XY spin chain are investigated in the presence of alternating the-nearest-neighbouring interaction of exchange couplings, external magnetic fields and the next-nearest neighbouring interaction. For a dimerised ferromagnetic spin chain, the NNNE appears only above a critical dimerized interaction, meanwhile, the dimerized interaction a effects a quantum phase transition point and improves the NNNE to a large extent. We also study the effect of ferromagnetic or antiferromagnetic next-nearest neighbouring (NNN) interaction on the dynamics of NNE and NNNE. The ferromagnetic NNN interaction increases and shrinks the NNE below and above a critical frustrated interaction respectively, while the antiferromagnetic NNN interaction always reduces the NNE. The antiferromagnetic NNN interaction results in a large value of NNNE compared with the case where the NNN interaction is ferromagnetic.

Keywords: the entanglement, alternating XY spin chain, the next-nearest neighbouring interactions

PACC: 0365, 7510H

1. Introduction

Entanglement is one of the most profound features of quantum mechanics and has been considered as an important resource in quantum information processing (QIP) including teleportation,[1] cryptography and secure direct communication,[2,3] and quantum communication and computation.[4] In order to realize quantum information process, a great effort has been made to generate the entanglement in linear optics,[5] cavity QED [6−8] and ion trap[9,10] schemes. In recent years much attention has been focused on the spin system with Heisenberg exchange interaction, which is a typical quantum system, and the entanglement properties have been extensively investigated in spin systems, such as Ising model[11] and isotropic and anisotropic Heisenberg models.[12−15] However, as far as we know, most of studies mentioned above merely focused on the models with the nearest neighbouring interaction of exchange couplings, while the next-nearest neighbouring interaction has not been taken into account. Dimerized systems and frustrated systems with the next-nearest-neighbouring (NNN) interactions[16−18] play an important role in condensed matter theory, and the entanglement properties of dimerized and frustrated systems has been considered.[19−23] Sun *et al*[19] investigated the entanglement properties of dimerized and frustrated spin-one models by applying the concept of negativity. In Ref.[20], entanglement is studied in an open alternating chain of nuclear spins $s = 1/2$ with spin–spin couplings in an external magnetic field under the thermodynamic equilibrium conditions. Gu *et al*[21] have investigated the entanglement in frustrated spin-half Heisenberg chains. Chen *et al*[22] analysed sublattice entanglement and quantum phase transitions in antiferromagnetic spin chains, Chen *et al*[23] studied the fidelity and quantum phase transition for the Heisenberg chain with next-nearest-neighbouring interaction. In fact, some one-dimensional and two-

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dimensional compounds ($CuGeO_3$ and NaV_2O_5) have manifested such interactions. Therefore, one should include the next-nearest neighbouring interaction in the study of spin chain entanglement.

The 1D Heisenberg model is simple but realistic and extensively studied in solid state systems. Recently, Osterloh *et al*[24] examined the entanglement between two spins of positions i and j in the spin chains for the pure case, Huang *et al*,[25] Osenda *et al*[26] and Shan *et al*[27] demonstrated that the entanglement can be controlled by introducing impurities into the systems. Meanwhile, the entanglement shares many features with quantum phase transition (QPT) for a many-body system.[28,29] The QPT, which occurs at an absolute zero temperature and is purely driven by quantum fluctuation, is the structural change in property of the ground state. The associated level crossings lead to the occurrence of non-analyticities in the energy spectrum. Therefore, the knowledge about the ground-state entanglement, the nonlocal correlation in quantum systems, is considered as a key to further understanding the QPT. In this paper, we study the pairwise ground state entanglement between the nearest-neighbouring sites and that between the next-nearest neighbouring sites in one-dimensional $s = \frac{1}{2}$ Heisenberg XY spin chain with dimerised exchange couplings and the next-nearest neighbouring coupling, which, to our knowledge, has not been reported before. The present study will help us further understand the behaviour of the entanglement and the QPT in one-dimensional alternating Heisenberg XY model with the next-nearest neighbouring interactions, and this model can display a variety of interesting physical phenomena. More interestingly, we can control or manipulate the NNE and the NNNE in QPT point with the help of dimerised exchange couplings, dimerized external magnetic fields and frustrated exchange interaction.

2. Solution of the XY model and spin–spin correlation functions

We consider a one-dimensional alternating Heisenberg XY model of N spin-$\frac{1}{2}$ particles with the nearest-neighbouring interactions and the next-nearest neighbouring interactions. One-dimensional Hamiltonian can be written as

$$\begin{aligned} H = &-\frac{1+\gamma}{2}\sum_{i=1}^{N} J_{i,i+1}\sigma_i^x\sigma_{i+1}^x \\ &-\frac{1-\gamma}{2}\sum_{i=1}^{N} J_{i,i+1}\sigma_i^y\sigma_{i+1}^y - \sum_{i=1}^{N} h_i\sigma_i^z \\ &-\frac{1+\gamma}{2}\sum_{i=1}^{N} J_{i,i+2}\sigma_i^x\sigma_{i+2}^x \\ &-\frac{1-\gamma}{2}\sum_{i=1}^{N} J_{i,i+2}\sigma_i^y\sigma_{i+2}^y, \end{aligned} \tag{1}$$

where $J_{i,i+1}$ and $J_{i,i+2}$ are alternating exchange interaction and the nearest-neighbouring interactions respectively, h_i is the strength of external magnetic field on site i, $\boldsymbol{\sigma}^{x,y,z}$ are the Pauli matrices, γ is a dimensionless parameter characterizing the anisotropy of the model, and N is the total number of sites. Furthermore, the periodic boundary conditions satisfy $\sigma_{N+1}^x = \sigma_1^x$, $\sigma_{N+1}^y = \sigma_1^y$, and $\sigma_{N+1}^z = \sigma_1^z$.

The spectrum of this Hamiltonian can be determined exactly by a straightforward application of the standard methods. The first step in the procedure is to perform a Jordan–Wigner transformation[30] by introducing Fermi operators c_j^+ and c_j, as a result, Hamiltonian (1) is mapped in the free fermion Hamiltonian

$$\begin{aligned} H = &-\sum_{i=1}^{N} J_{i,i+1}[(c_i^+c_{i+1} + \gamma c_i^+c_{i+1}^+) + \text{h.c}] \\ &-2\sum_{i=1}^{N} h_i\left(c_i^+c_i - \frac{1}{2}\right) \\ &-\sum_{i=1}^{N} J_{i,i+2}[(c_i^+c_{i+2} + \gamma c_i^+c_{i+2}^+) + \text{h.c}]. \end{aligned} \tag{2}$$

In this paper, the exchange interaction and the external magnetic field have the forms $J_{2i-1,2i} = J_1 = J$, $J_{2i,2i+1} = J_2 = \alpha J$, $h_{2i,2i+1} = h_{2i-1,2i}(h) = \beta h$, $(i = 1, 2, \ldots, \frac{N}{2})$ respectively, where $\alpha = J_2/J_1$ introduces the dimerised parameter, the ratio of the next-nearest ($J_{i,i+2} = J_3$) to the nearest-neighbouring interaction coefficients, $\kappa = J_3/J_1$, is called the frustration parameter. $J < 0$ and $J > 0$ correspond to the antiferromagnetic and the ferromagnetic cases, respectively. For $J_3 = 0$, expression (2) reduces to one-dimensional alternating(dimerised) Heisenberg model, and for $J_1 = J_2$ it reduces to one-dimensional frustrated Heisenberg model.

The density-matrix renormalization-group (DMRG) method[31,32] is applied to obtaining the spin correlation function. The two-point reduced density matrix obtained by tracing the full density matrix of the system over all sites except the pair $\{i, j\}$ has the form

$$\rho_{i,j} = \frac{1}{4}\Big(I_{i,j} + \langle\sigma_i^z\rangle\sigma_i^z + \langle\sigma_j^z\rangle\sigma_j^z + \sum_{k=x,y,z}\langle\sigma_i^k\sigma_j^k\rangle\sigma_i^k\sigma_j^k\Big). \quad (3)$$

In this part, we choose the concurrence defined by Wootters[33] as a measure of the pairwise entanglement. For a pure or mixed state of two qubits described by the density matrix $\boldsymbol{\rho}$, the concurrence C may be calculated explicitly as

$$C(\boldsymbol{\rho}) = \max(0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4), \quad (4)$$

where λ_1, λ_2, λ_3, and λ_4 are the eigenvalues in descending order of the spin-flipped density operator R, which is defined as $R = \sqrt{\sqrt{\rho}\tilde{\rho}\sqrt{\rho}}$, where $\tilde{\rho} = (\sigma_y \otimes \sigma_y)\rho^*(\sigma_y \otimes \sigma_y)$, $\tilde{\rho}$ denotes the complex conjugate of ρ and σ_y is the usual Pauli matrix. All the matrix elements in the density matrix can be calculated from the different spin–spin correlation functions.

3. Results and discussion

In this paper, we focus on the discussion of transverse Ising model with $\gamma = 1$ and the introduction of the dimensionless parameter $\lambda = J/(2h)$. The goal of our present study is to find out dynamic characteristics of the entanglement in varying the dimerised parameters of exchange couplings, external magnetic fields and NNN interaction. Figure 1 displays the diagram of the $J_1 - J_2 - J_3$ model which can be considered either as a linear chain(a) or a zigzag chain(b). The alternating the nearest-neighbouring interaction is J_1 and J_2 respectively, while the next-nearest-neighbouring interaction is parametrized by J_3. We consider three different physical models, i.e. dimerised ferromagnetic spin chain, frustrated ferromagnetic–ferromagnetic (F–F) spin chain, and frustrated ferromagnetic–antiferromagnetic (F–AF) spin chain. First, we examine the dimerised Heisenberg chain. This model is characterized by an alternation of strong and weak bonds between two nearest-neighbouring spins.

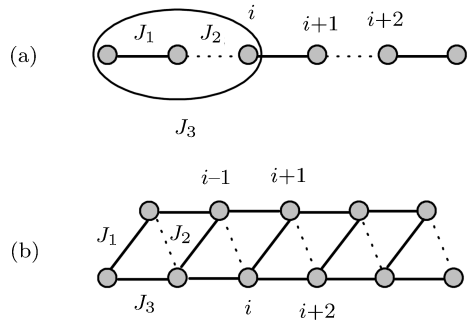


Fig.1. Diagram of the $J_1 - J_2 - J_3$ model that can be considered either as a linear chain(a) or a zigzag chain(b). The nearest-neighbouring alternating interaction is J_1 and J_2 respectively, while the next-nearest-neighbouring interaction is parametrized by J_3.

Figure 2 shows the nearest neighbouring concurrence $C(1,2)$ and $C(2,3)$, which correspond to two nearest-neighbouring spins coupled by bonds J_1 and J_2 respectively, as a function of the reduced coupling constant λ at different values of the dimerised parameter α of exchange coupling, parameter β of external magnetic field with the system size N=59. Numerical results in Figs.2(a) and 2(c) show that the concurrence $C(1,2)$ decreases when the dimerised parameter α of exchange couplings increases, while for the concurrence $C(2,3)$ the situation is opposite, and the pair of qubits (1,2) and (2,3) has the same pairwise entanglement for the homogeneous chain $\alpha = 1$. In fact, in the case of weak alternation of the nearest-neighbouring exchange coupling, we have here the dimerised spin chain which can be considered qualitatively as a set of non-interacting spin pairs. In the limit of strong dimerization, the concurrence reaches a maximum value. Moreover, spin 2 can be entangled both with spin 1 and with spin 3. Since spin 2 is strongly entangled with spin 1, the entanglement of spins 2 and 3 is weaker. Obviously, the increase of exchange interaction J_2 suppresses the entanglement of spins coupled by J_1. The increase of J_2 can enhance the entanglement between spins coupled by J_2. This explains the behaviour of the concurrence displayed in Fig.2. The effect of the alternation of external magnetic field β is also shown in Figs.2(b) and 2(d). However, different from the effect of the exchange couplings, the concurrences (1,2) and (2,3) have a similar behaviour and increase first and then decrease with the increase of the value of parameter β, suggesting a critical alternation of external magnetic field β_c, where the maximum concurrence takes place, must exist.

From Fig.2, we can see that the alternate interaction plays an important role in enhancing the nearest neighbouring concurrence. The maximum value of the concurrence between neighbouring sites does not occur at the critical point. This is because based on the properties of shared entanglement this maximum should occur away from the critical point. Entanglement sharing is relevant to the quantum phase transition in the transverse Ising model, for it sets a fundamental bound to the amount of entanglement that may be distributed among the other sites, which means that as the overall entanglement in the lattice is increased, some sites become disentangled. However, is well all known, the maximum value of the concurrence between the next-nearest-neighbouring sites does occur at the critical point $\lambda = 1$, so it is necessary to discuss in this subsection the effect on the next-nearest-neighbouring entanglement (NNNE).

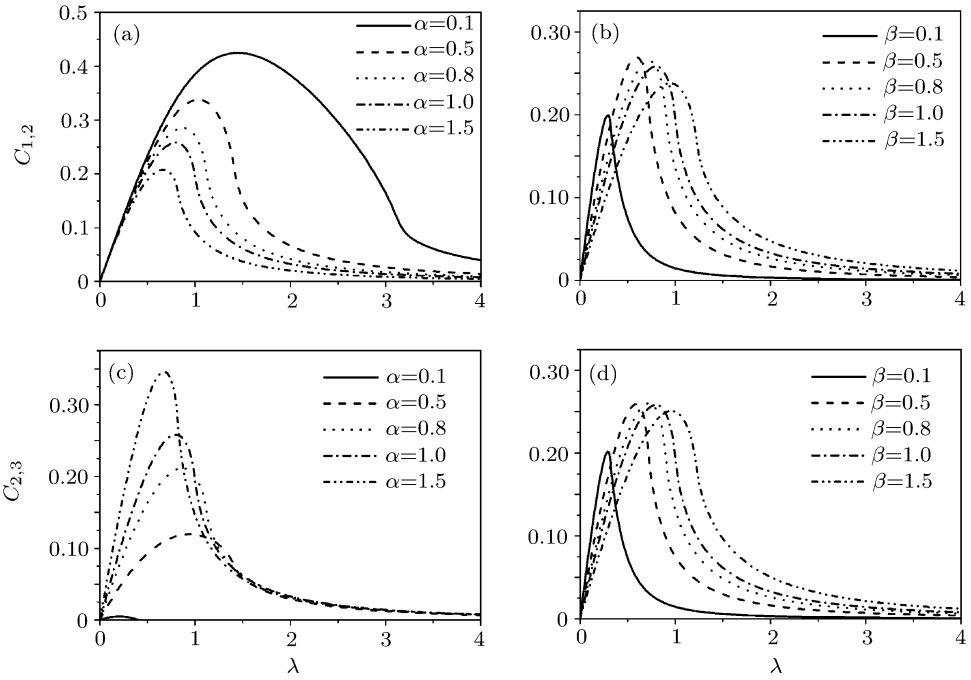


Fig.2. The nearest neighbouring concurrence $C_{1,2}$ and $C_{2,3}$ as a function of reduced coupling constant λ for various alternating values of the nearest-neighbouring interaction and external magnetic field, with the NNN interaction $\kappa = 0$.

Figures 3(a) and 3(b) show the change of concurrence $C(1,3)$ as a function of λ for different values of alternate interactions α and β with $\kappa = 0$, i.e. in the absence of the NNN interaction. We can see that there is no entanglement at $\alpha = 0.5$ and $\beta = 0.5$. The weak alternate interactions α and β suppress and finally completely destroy the NNN concurrence. The dashed line in Fig.3(a) depicts that at the critical point, $\lambda = 1$, of the transverse Ising model ($\alpha = 1$), where maximum next-nearest-neighbouring entanglement occurs, there is a fundamental transition in the structure of the ground state. This is consistent with the previous result. As α increases the NNN concurrence tends to increase faster, the peak value induced by the NN interaction increases and the λ_m, where concurrence approaches a maximum, shifts to the left very rapidly. The dimerised interaction does facilitate the formation of entanglement because of the inner alternation. Therefore, we can further understand the relation between the entanglement and the quantum transition. In Figs.3(c) and 3(d), we plot our numerical results for the threshold NN alternate interactions α and β for the case of next-nearest-neighbouring concurrence. Only above the critical α and β, can the NNN concurrence appears.

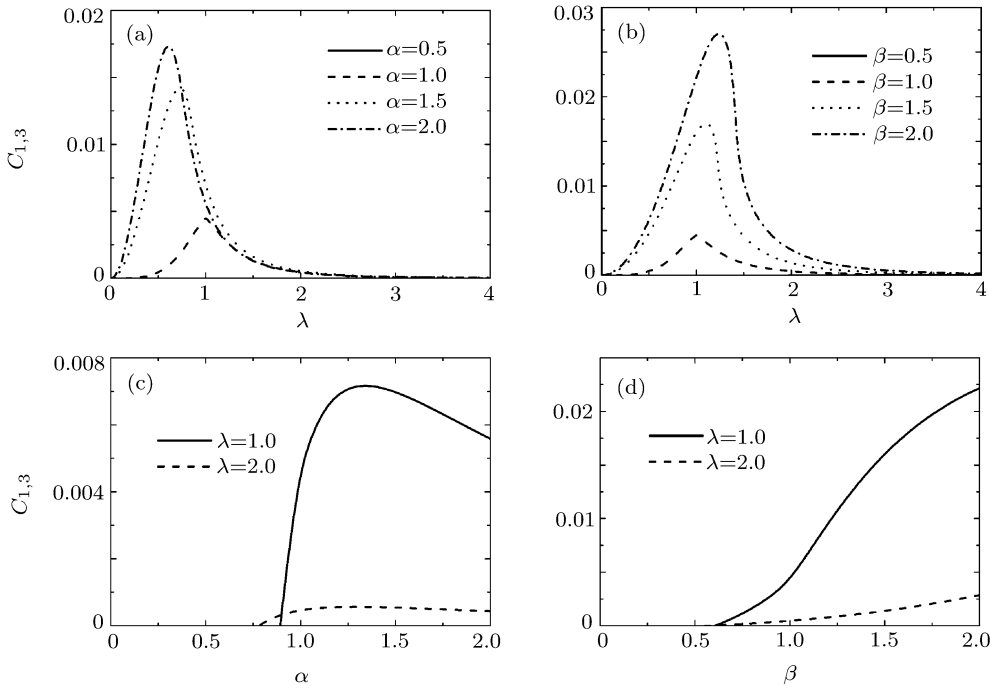


Fig.3. The next-nearest-neighbouring concurrence $C_{1,3}$ as a function of reduced coupling constant λ for various alternating values of the nearest-neighbouring interaction and external magnetic field, with the NNN interaction $\kappa = 0$.

For the frustrated model, there is a competition between the NN and the NNN interactions. So the model displays some special features of entanglement. In Fig.4, we give the results of the NN and the NNN concurrence as a function of parameter λ for different values of frustrated interaction κ. The NNN interaction has a different frustration effect on $C(1,2)$. For a frustrated ferromagnetic–ferromagnetic (F–F) spin chain $\kappa > 0$, by making a comparison among the different curves in Fig.4(a), it is interesting to find that the entanglement peak between the nearest neighbours in the dotted line increases to a value larger than that in the solid line. With the increasing of κ, the concurrence indicated by the dash-dotted line decreases. We can imagine that there must exist a critical frustration strength (κ_c): below κ_c, the NNN interaction enhances entanglement, while above κ_c, the NNN interaction shrinks the entanglement. This behaviour is due to the energy level crossing at the point $\kappa = 0.5$, as seen clearly from Fig.4(a). Before and after the critical point, the entanglements display distinct behaviours. However, for a frustrated ferromagnetic–antiferromagnetic (F–AF) spin chain $\kappa < 0$, the situation becomes different due to the frustration, with the increase of absolute value of κ and weak parameter λ, antiferromagnetic NNN interaction always shrinks the entanglement, which is different from the results obtained from Fig.4(a). Another important character revealed from Fig.4(b) is that, as parameter λ increases, the concurrence increases and tends to move to infinity (> 0) by increasing the value of parameter κ: the strong κ is helpful for keeping the better entanglement. It is the frustrated interaction that leads to considerably different evolutions of the entanglement, hence the entanglement is rather sensitive to any variation in NNN interaction. From Figs.4(c) and 4(d), we can see that the height of the peak increases with the increase of antiferromagnetic κ, which is a characteristic feature of one-dimensional Heisenberg antiferromagnetic chain. This suggests that the antiferromagnetic component becomes significant for large values of κ. Meanwhile, the antiferromagnetic NNN interaction results in a large value of NNNE compared with the case where the NNN interaction is ferromagnetic. In order to explain these results it is necessary to take into account the influence of the competing roles played by the NN and the NNN interactions on the entangled states. Thus, by adjusting the NNN interaction constant, one can control or manipulate the NN and the NNN entanglements.

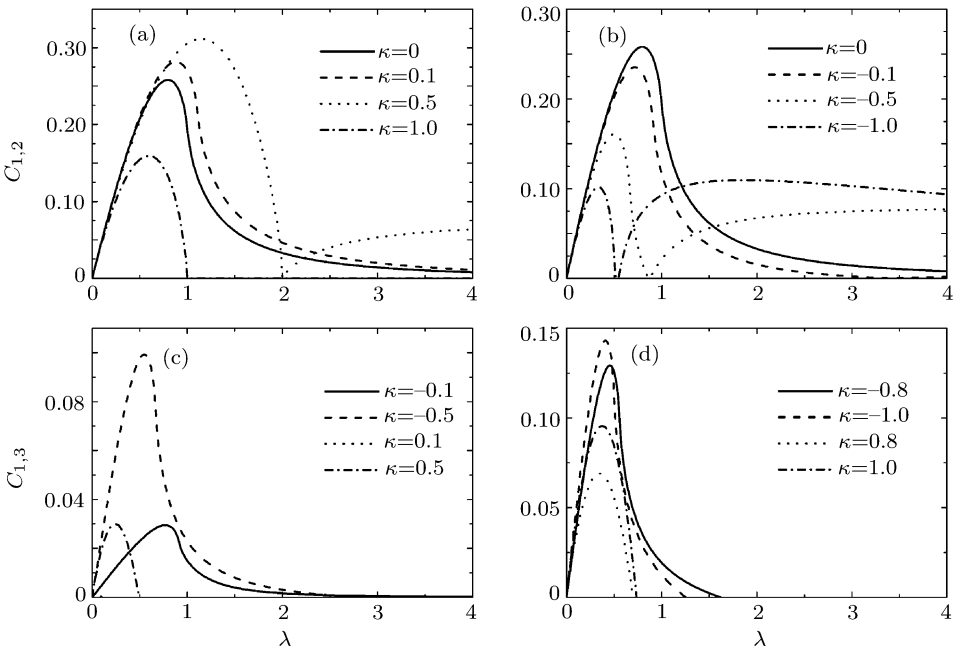


Fig.4. The concurrences $C_{1,2}$ and $C_{1,3}$ as a function of reduced coupling constant λ for various frustrated values of next-nearest-neighbouring interaction, with the NN interaction $\alpha = \beta = 1.0$.

4. Conclusions

From the above analysis, it is clearly noted that dimerised exchange couplings, dimerised external magnetic fields and frustrated exchange interaction, which play the competing roles in enhancing quantum entanglement, have a notable influence on the NN and the NNN concurrences in one-dimensional $s = \frac{1}{2}$ XY spin system. The NN and the NNN concurrences exhibit some interesting phenomena. For a dimerised ferromagnetic spin chain, the NNNE appears only above the critical dimerised interaction, which a effects quantum phase transition point and increases the NNNE. For a ferromagnetic-antiferromagnetic frustrated spin chain, the NNN interaction is predominant in the competing role and can enhance the entanglement to a steady value. The ferromagnetic NNN interaction increases and shrinks the NNE below and above critical frustrated interaction respectively, while the antiferromagnetic NNN interaction always reduces the NNE. Meanwhile, the antiferromagnetic NNN interaction can generate a larger value of NNNE compared with the case where the NNN interaction is ferromagnetic. So we can employ the NNN interaction strength as well as dimerised interaction to realize the quantum entanglement control. As for the case where $\gamma \neq 1$ (XY model), we will present further reports in the future.

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